Carbamothioic acid, bis(1-methylethyl)-, S-(2,3-dichloro-2-propenyl) ester

Other names: 2,3-DCDT
2,3-Dichlorallyl-N,N-(diisopropyl)-thiocarbamate
2,3-Dichloro-2-propene-1-thiol, diisopropylcarbamate
2,3-Dichloroallyl N,N-diisopropylthiolcarbamate
2-Propene-1-thiol, 2,3-dichloro-, diisopropylcarbamate
Avadex
Avadex I
Avadex II
Bis(1-methylethyl) carbamothioic acid, S-(2,3-dichloro-2-propenyl)ester
CP 15,336
CP 15336
Carbamic acid, diisopropylthio-, S-(2,3-dichloroallyl) ester
DATC
Di-isopropylthiolocarbamate de S-(2,3-dichloro allyle)
Diallaat
Diallat
Diallate
Dichloroallyl diisopropylthiocarbamate
Diisopropylthiocarbamic acid, S-(2,3-dichloroallyl) ester
Pyradex
Rcra waste number U062
S-(2,3-Dichlor-allyl)-N,N-diisopropyl-monothiocarbamaat
S-(2,3-Dichloro-allil)-N,N-diisopropil-monotiocarbammato
S-(2,3-Dichloroallyl) Diisopropylthiocarbamate

Inchi: InChI=1S/C10H17Cl2NOS/c1-7(2)13(8(3)4)10(14)15-6-9(12)5-11/h5,7-8H,6H2,1-4H3/b9

InchiKey: SPANOECCGNXGNR-UITAMQMPSA-N

Formula: C10H17Cl2NOS

SMILES: CC(C)N(C(=O)SCC(Cl)=CCl)C(C)C

Mol. weight [g/mol]: 270.22

CAS: 2303-16-4

Physical Properties

Property code	Value	Unit	Source
gf	91.23	kJ/mol	Joback Method
hf	-187.52	kJ/mol	Joback Method
hfus	30.65	kJ/mol	Joback Method

hvap	61.49	kJ/mol	Joback Method
log10ws	-4.29		Estimated Solubility Method
logp	4.277		Crippen Method
mcvol	199.840	ml/mol	McGowan Method
pc	2265.42	kPa	Joback Method
rinpol	1702.00		NIST Webbook
rinpol	1713.00		NIST Webbook
rinpol	1720.00		NIST Webbook
rinpol	287.02		NIST Webbook
rinpol	285.04		NIST Webbook
rinpol	1704.00		NIST Webbook
tb	641.31	K	Joback Method
tc	857.18	K	Joback Method
tf	330.06	K	Joback Method
vc	0.741	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.54	J/mol×K	641.31	Joback Method
cpg	486.39	J/mol×K	677.29	Joback Method
cpg	499.32	J/mol×K	713.27	Joback Method
cpg	511.40	J/mol×K	749.25	Joback Method
cpg	522.66	J/mol×K	785.22	Joback Method
cpg	533.15	J/mol×K	821.20	Joback Method
cpg	542.93	J/mol×K	857.18	Joback Method

Sources

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2303164&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume